

organic compounds



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1-[3-(4-Methylphenyl)-5-[5-(2-nitrophenyl)furan-2-yl]-4,5-dihydro-1H-pyrazol-1-yl]ethanone

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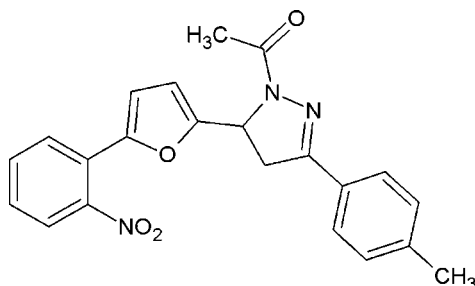
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.084; wR factor = 0.242; data-to-parameter ratio = 11.6.

In the title compound, $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_4$, the dihedral angle between the furan and pyrazole rings is 82.73 (19)° while the dihedral angles between the furan and pyrazole rings and their attached benzene rings are 31.93 (18) and 1.88 (18)°, respectively. In the crystal, inversion dimers linked by pairs of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds generate $R_2^2(16)$ loops. In addition, weak $\text{C}-\text{H}\cdots\pi$ and aromatic $\pi-\pi$ stacking [minimum centroid-centroid distance = 3.5374 (17) Å] interactions are observed.

Related literature

For background to the biological properties of pyrazole derivatives, see: Amir *et al.* (2008); Husain *et al.* (2008).



Experimental

Crystal data

 $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_4$ $M_r = 389.40$

Triclinic, $P\bar{1}$
 $a = 7.6235$ (3) Å
 $b = 10.5652$ (4) Å
 $c = 13.1177$ (4) Å
 $\alpha = 103.344$ (2)°
 $\beta = 95.025$ (2)°
 $\gamma = 108.221$ (2)°

$V = 961.78$ (6) Å³
 $Z = 2$
 $\text{Cu } K\alpha$ radiation
 $\mu = 0.78$ mm⁻¹
 $T = 296$ K
 $0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker X8 Proteum CCD
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2013)
 $T_{\min} = 0.842$, $T_{\max} = 0.854$

10640 measured reflections
 3083 independent reflections
 2186 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.138$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.084$
 $wR(F^2) = 0.242$
 $S = 1.06$
 3083 reflections

265 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.38$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg4 is the centroid of the C23–C28 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C14}-\text{H14}\cdots\text{O19}^{\text{i}}$	0.93	2.56	3.462 (4)	162
$\text{C18}-\text{H18C}\cdots\text{Cg4}^{\text{ii}}$	0.96	2.69	3.595 (4)	158

Symmetry codes: (i) $-x, -y, -z + 2$; (ii) $-x, -y, -z + 1$.

Data collection: APEX2 (Bruker, 2013); cell refinement: SAINT (Bruker, 2013); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7133).

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supplementary materials

Acta Cryst. (2013). E69, o1528 [doi:10.1107/S1600536813024690]

1-{3-(4-Methylphenyl)-5-[5-(2-nitrophenyl)furan-2-yl]-4,5-dihydro-1H-pyrazol-1-yl}ethanone

N. Vinutha, S. Madan Kumar, B. S. Vidyashree Jois, Kalluraya Balakrishna, N. K. Lokanath and D. Revannasiddaiah

1. Comment

The ongoing work in our lab for synthesizing pyrazoline derivatives resulted the title molecule. Similar compounds are used for the preparation of drugs in the pharmacological industries (Amir *et al.*, 2008; Husain *et al.*, 2008).

In the title compound (Fig. 1), the pyrazole ring makes a dihedral angle of 82.73 (19)°, 88.84 (18)° and 1.88 (18)° with furan, nitrophenyl and terminal methylphenyl rings, respectively. The furan ring makes a dihedral angle of 82.35 (18)° and 31.93 (18)° with methyl phenyl and nitrophenyl rings, respectively. The dihedral angle between terminal nitrophenyl and methylphenyl ring is 88.23 (17)°.

The title molecules are linked to one another with C14—H14···O19 intermolecular hydrogen bonds with $R_2^2(16)$ ring motif (Fig. 2 and Table 1). In addition, short contacts C—H··· π (Cg4) with distance 3.595 (4) Å (angle 158°) [$-x, -y, z - 1$]. And π ··· π between Cg2 and Cg1 with distance 3.5374 (17)° [x, y, z] and between Cg2 and Cg4 with a distance 3.641 (2)° [$x - 1, -y, z - 1$] were observed, where Cg1:O11/C10/C14/C13/C12, Cg2:N16/N20/C21/C22/C15 and Cg4:C23/C24/C25/C26/C27/C28.

2. Experimental

A mixture of 4-methylphenyl-3-[5-(2-nitrophenyl)furan-2-yl]prop-2-en-1-one (10 mmol), hydrazine hydrate (50 mmol) and glacial acetic acid (40 ml) were refluxed for 24 h. The resulting mixture was poured into water (100 ml) and allowed to stand. The precipitate that formed was separated by filtration, washed with cold water and then recrystallized from mixed DMF-ethanol solvents to yield brown blocks.

3. Refinement

All the H atoms were fixed geometrically (C—H = 0.93–0.96 Å) and allowed to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and $= 1.2U_{\text{eq}}(\text{C})$ for other H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELX:97* (Sheldrick, 2008).

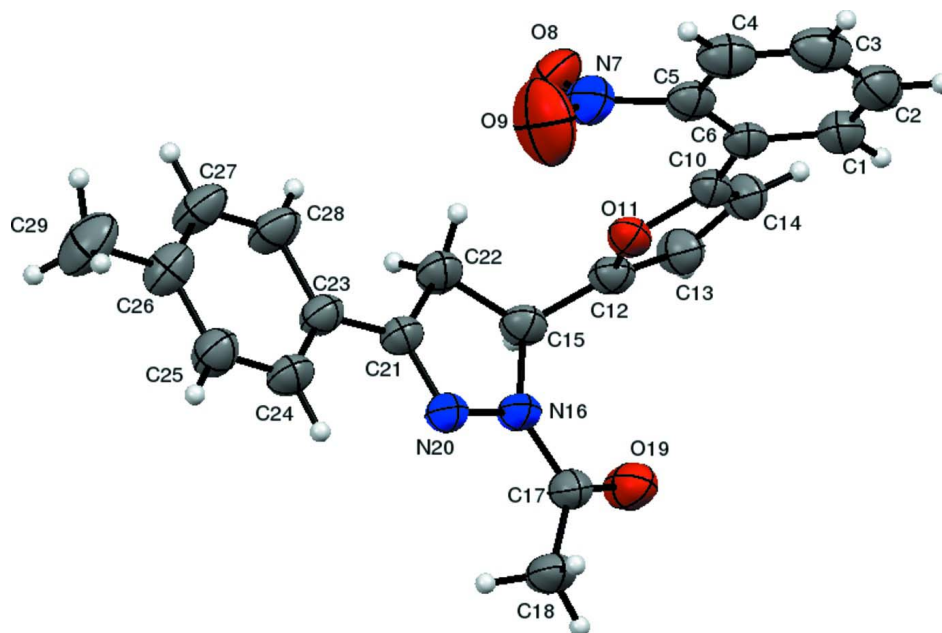
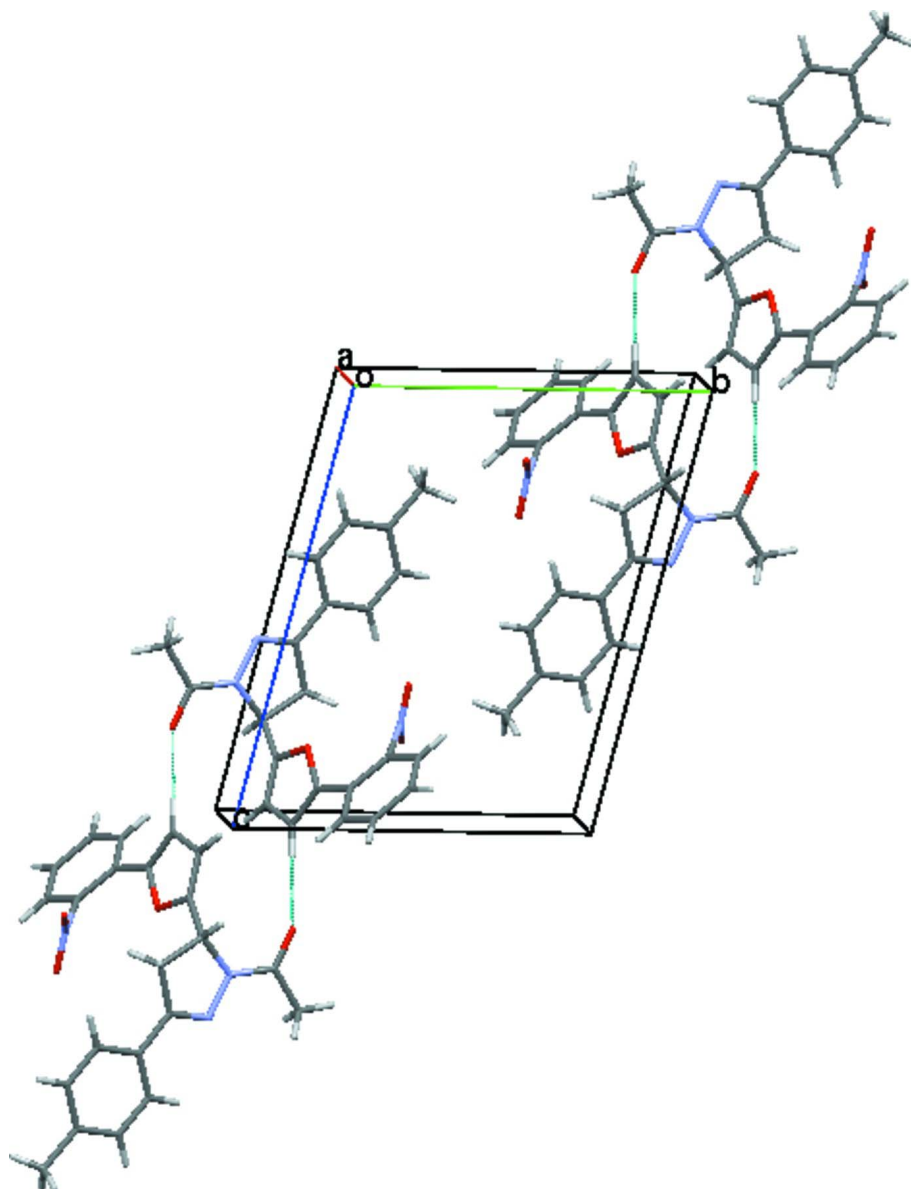


Figure 1

ORTEP diagram of the title compound with 50% probability ellipsoids.

**Figure 2**

Packing diagram of molecule, viewed along the crystallographic *a* axis. Dotted lines represent hydrogen bonds.

1-{3-(4-Methylphenyl)-5-[5-(2-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone

Crystal data

$C_{22}H_{19}N_3O_4$

$M_r = 389.40$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.6235\ (3)\ \text{\AA}$

$b = 10.5652\ (4)\ \text{\AA}$

$c = 13.1177\ (4)\ \text{\AA}$

$\alpha = 103.344\ (2)^\circ$

$\beta = 95.025\ (2)^\circ$

$\gamma = 108.221\ (2)^\circ$

$V = 961.78\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 408$

$D_x = 1.345\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54178\ \text{\AA}$

Cell parameters from 3083 reflections

$\theta = 3.5\text{--}64.8^\circ$

$\mu = 0.78\ \text{mm}^{-1}$

$T = 296$ K
Block, brown

$0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker X8 Proteum CCD
diffractometer
Radiation source: Bruker MicroStar microfocus
rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 pixels mm^{-1}
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2013)

$T_{\min} = 0.842$, $T_{\max} = 0.854$
10640 measured reflections
3083 independent reflections
2186 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.138$
 $\theta_{\max} = 64.8^\circ$, $\theta_{\min} = 3.5^\circ$
 $h = -8 \rightarrow 8$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.084$
 $wR(F^2) = 0.242$
 $S = 1.06$
3083 reflections
265 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods
Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1607P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.40$ e \AA^{-3}
 $\Delta\rho_{\min} = -0.38$ e \AA^{-3}
Extinction correction: *SHELXL97* (Sheldrick,
2008), $\text{FC}^* = \text{KFC}[1 + 0.001\text{XFC}^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
Extinction coefficient: 0.018 (3)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O8	0.2462 (4)	0.4170 (3)	0.8072 (2)	0.0736 (10)
O9	0.0362 (6)	0.3831 (5)	0.6738 (2)	0.1186 (18)
O11	0.1066 (3)	0.1532 (2)	0.82063 (14)	0.0429 (7)
O19	0.0746 (4)	-0.2396 (2)	0.77708 (19)	0.0647 (9)
N7	0.0831 (5)	0.3916 (3)	0.7666 (2)	0.0603 (11)
N16	0.1731 (4)	-0.0929 (2)	0.67816 (18)	0.0445 (8)
N20	0.1833 (4)	-0.0661 (2)	0.57957 (19)	0.0423 (8)
C1	-0.2096 (5)	0.2889 (3)	0.9665 (3)	0.0561 (11)
C2	-0.3242 (5)	0.3645 (4)	0.9620 (3)	0.0652 (14)
C3	-0.3090 (5)	0.4456 (4)	0.8924 (3)	0.0649 (14)
C4	-0.1778 (5)	0.4506 (3)	0.8273 (3)	0.0587 (11)
C5	-0.0621 (4)	0.3744 (3)	0.8330 (2)	0.0469 (10)

C6	−0.0729 (4)	0.2910 (3)	0.9021 (2)	0.0418 (9)
C10	0.0452 (4)	0.2079 (3)	0.9105 (2)	0.0425 (9)
C12	0.2155 (4)	0.0806 (3)	0.8501 (2)	0.0415 (9)
C13	0.2212 (5)	0.0893 (3)	0.9544 (2)	0.0497 (11)
C14	0.1110 (5)	0.1697 (3)	0.9934 (2)	0.0505 (11)
C15	0.3075 (4)	0.0204 (3)	0.7665 (2)	0.0447 (10)
C17	0.0708 (5)	−0.2192 (3)	0.6880 (2)	0.0472 (11)
C18	−0.0432 (5)	−0.3260 (3)	0.5893 (3)	0.0592 (11)
C21	0.3124 (4)	0.0530 (3)	0.5932 (2)	0.0414 (9)
C22	0.4090 (4)	0.1216 (3)	0.7063 (2)	0.0502 (10)
C23	0.3564 (4)	0.1109 (3)	0.5040 (2)	0.0440 (10)
C24	0.2619 (4)	0.0440 (3)	0.4011 (3)	0.0487 (10)
C25	0.3054 (5)	0.1030 (3)	0.3190 (3)	0.0539 (12)
C26	0.4428 (5)	0.2314 (4)	0.3360 (3)	0.0556 (12)
C27	0.5380 (5)	0.2980 (4)	0.4389 (3)	0.0628 (12)
C28	0.4980 (5)	0.2405 (3)	0.5222 (3)	0.0565 (11)
C29	0.4863 (6)	0.2965 (5)	0.2462 (4)	0.0812 (17)
H1	−0.22270	0.23450	1.01380	0.0670*
H2	−0.41350	0.36140	1.00620	0.0780*
H3	−0.38780	0.49690	0.88980	0.0780*
H4	−0.16700	0.50470	0.77980	0.0700*
H13	0.28560	0.04970	0.99370	0.0600*
H14	0.08830	0.19190	1.06270	0.0610*
H15	0.39680	−0.01490	0.79860	0.0540*
H18A	−0.08350	−0.41510	0.60300	0.0890*
H18B	0.03140	−0.32780	0.53400	0.0890*
H18C	−0.15080	−0.30380	0.56720	0.0890*
H22A	0.39530	0.21130	0.73180	0.0600*
H22B	0.54140	0.13360	0.71370	0.0600*
H24	0.16790	−0.04200	0.38710	0.0580*
H25	0.24060	0.05540	0.25040	0.0650*
H27	0.63170	0.38400	0.45230	0.0750*
H28	0.56480	0.28760	0.59050	0.0680*
H29A	0.37170	0.28030	0.20040	0.1220*
H29B	0.56460	0.25620	0.20630	0.1220*
H29C	0.55040	0.39440	0.27470	0.1220*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O8	0.0562 (17)	0.0598 (16)	0.093 (2)	0.0000 (13)	0.0194 (14)	0.0235 (14)
O9	0.146 (3)	0.173 (4)	0.052 (2)	0.063 (3)	0.025 (2)	0.045 (2)
O11	0.0469 (13)	0.0401 (11)	0.0322 (11)	0.0069 (9)	0.0038 (9)	0.0041 (9)
O19	0.0872 (19)	0.0492 (14)	0.0484 (15)	0.0091 (12)	0.0117 (12)	0.0156 (11)
N7	0.074 (2)	0.0525 (17)	0.0494 (18)	0.0117 (15)	0.0152 (15)	0.0165 (13)
N16	0.0507 (16)	0.0337 (13)	0.0352 (14)	0.0011 (11)	0.0061 (11)	0.0024 (10)
N20	0.0471 (15)	0.0354 (13)	0.0372 (14)	0.0060 (11)	0.0074 (11)	0.0073 (10)
C1	0.053 (2)	0.0454 (18)	0.058 (2)	0.0071 (16)	0.0147 (16)	0.0032 (15)
C2	0.046 (2)	0.055 (2)	0.076 (3)	0.0071 (17)	0.0142 (17)	−0.0045 (18)
C3	0.049 (2)	0.052 (2)	0.077 (3)	0.0146 (17)	−0.0064 (19)	−0.0037 (18)

C4	0.054 (2)	0.0459 (19)	0.062 (2)	0.0099 (16)	−0.0063 (17)	0.0042 (16)
C5	0.0431 (18)	0.0403 (16)	0.0397 (17)	0.0005 (14)	−0.0028 (13)	0.0006 (13)
C6	0.0390 (17)	0.0326 (15)	0.0387 (16)	0.0003 (12)	0.0022 (12)	−0.0003 (12)
C10	0.0443 (17)	0.0364 (15)	0.0343 (16)	0.0024 (13)	0.0076 (12)	0.0017 (12)
C12	0.0425 (17)	0.0342 (15)	0.0372 (16)	0.0050 (13)	−0.0002 (12)	0.0034 (12)
C13	0.061 (2)	0.0467 (18)	0.0371 (18)	0.0125 (16)	0.0043 (14)	0.0129 (14)
C14	0.065 (2)	0.0474 (18)	0.0332 (17)	0.0101 (16)	0.0105 (14)	0.0116 (13)
C15	0.0438 (18)	0.0418 (16)	0.0360 (17)	0.0050 (13)	−0.0009 (13)	0.0035 (13)
C17	0.056 (2)	0.0347 (16)	0.0447 (19)	0.0083 (14)	0.0122 (14)	0.0079 (13)
C18	0.067 (2)	0.0382 (17)	0.052 (2)	−0.0020 (16)	0.0078 (17)	0.0026 (15)
C21	0.0368 (16)	0.0359 (15)	0.0432 (17)	0.0043 (12)	0.0065 (12)	0.0066 (12)
C22	0.0432 (18)	0.0457 (17)	0.0453 (19)	−0.0002 (14)	0.0049 (13)	0.0037 (14)
C23	0.0371 (17)	0.0373 (15)	0.0501 (19)	0.0035 (13)	0.0059 (13)	0.0111 (13)
C24	0.0404 (17)	0.0403 (16)	0.052 (2)	0.0003 (13)	0.0050 (14)	0.0070 (14)
C25	0.050 (2)	0.054 (2)	0.048 (2)	0.0048 (16)	0.0060 (15)	0.0147 (15)
C26	0.045 (2)	0.057 (2)	0.064 (2)	0.0092 (16)	0.0070 (15)	0.0276 (17)
C27	0.048 (2)	0.052 (2)	0.072 (2)	−0.0072 (16)	0.0014 (17)	0.0230 (18)
C28	0.0463 (19)	0.0471 (18)	0.056 (2)	−0.0073 (15)	−0.0026 (15)	0.0128 (15)
C29	0.076 (3)	0.082 (3)	0.083 (3)	0.006 (2)	0.011 (2)	0.048 (2)

Geometric parameters (Å, °)

O8—N7	1.229 (5)	C23—C28	1.406 (5)
O9—N7	1.213 (4)	C24—C25	1.379 (5)
O11—C10	1.376 (3)	C25—C26	1.385 (5)
O11—C12	1.381 (4)	C26—C27	1.384 (5)
O19—C17	1.236 (4)	C26—C29	1.507 (6)
N7—C5	1.461 (5)	C27—C28	1.380 (5)
N16—N20	1.390 (3)	C1—H1	0.9300
N16—C15	1.487 (4)	C2—H2	0.9300
N16—C17	1.361 (4)	C3—H3	0.9300
N20—C21	1.294 (4)	C4—H4	0.9300
C1—C2	1.362 (6)	C13—H13	0.9300
C1—C6	1.396 (5)	C14—H14	0.9300
C2—C3	1.378 (6)	C15—H15	0.9800
C3—C4	1.367 (6)	C18—H18A	0.9600
C4—C5	1.376 (5)	C18—H18B	0.9600
C5—C6	1.393 (4)	C18—H18C	0.9600
C6—C10	1.454 (4)	C22—H22A	0.9700
C10—C14	1.353 (4)	C22—H22B	0.9700
C12—C13	1.346 (4)	C24—H24	0.9300
C12—C15	1.480 (4)	C25—H25	0.9300
C13—C14	1.418 (5)	C27—H27	0.9300
C15—C22	1.531 (4)	C28—H28	0.9300
C17—C18	1.490 (5)	C29—H29A	0.9600
C21—C22	1.499 (4)	C29—H29B	0.9600
C21—C23	1.458 (4)	C29—H29C	0.9600
C23—C24	1.383 (5)		
C10—O11—C12	106.9 (2)	C27—C26—C29	121.3 (4)

O8—N7—O9	123.2 (4)	C26—C27—C28	121.9 (4)
O8—N7—C5	119.1 (3)	C23—C28—C27	120.1 (3)
O9—N7—C5	117.7 (4)	C2—C1—H1	119.00
N20—N16—C15	113.1 (2)	C6—C1—H1	119.00
N20—N16—C17	121.9 (2)	C1—C2—H2	120.00
C15—N16—C17	124.3 (2)	C3—C2—H2	120.00
N16—N20—C21	108.1 (2)	C2—C3—H3	120.00
C2—C1—C6	121.8 (3)	C4—C3—H3	120.00
C1—C2—C3	120.5 (4)	C3—C4—H4	120.00
C2—C3—C4	119.9 (4)	C5—C4—H4	120.00
C3—C4—C5	119.0 (3)	C12—C13—H13	126.00
N7—C5—C4	116.3 (3)	C14—C13—H13	126.00
N7—C5—C6	120.8 (3)	C10—C14—H14	127.00
C4—C5—C6	122.9 (3)	C13—C14—H14	127.00
C1—C6—C5	115.9 (3)	N16—C15—H15	109.00
C1—C6—C10	119.2 (3)	C12—C15—H15	109.00
C5—C6—C10	124.9 (3)	C22—C15—H15	109.00
O11—C10—C6	118.5 (2)	C17—C18—H18A	109.00
O11—C10—C14	109.5 (3)	C17—C18—H18B	109.00
C6—C10—C14	132.0 (3)	C17—C18—H18C	109.00
O11—C12—C13	109.3 (3)	H18A—C18—H18B	109.00
O11—C12—C15	116.1 (2)	H18A—C18—H18C	110.00
C13—C12—C15	134.5 (3)	H18B—C18—H18C	109.00
C12—C13—C14	107.5 (3)	C15—C22—H22A	111.00
C10—C14—C13	106.8 (2)	C15—C22—H22B	111.00
N16—C15—C12	113.3 (3)	C21—C22—H22A	111.00
N16—C15—C22	101.4 (2)	C21—C22—H22B	111.00
C12—C15—C22	114.1 (3)	H22A—C22—H22B	109.00
O19—C17—N16	119.2 (3)	C23—C24—H24	120.00
O19—C17—C18	123.3 (3)	C25—C24—H24	120.00
N16—C17—C18	117.5 (2)	C24—C25—H25	119.00
N20—C21—C22	114.0 (2)	C26—C25—H25	119.00
N20—C21—C23	121.3 (2)	C26—C27—H27	119.00
C22—C21—C23	124.7 (3)	C28—C27—H27	119.00
C15—C22—C21	103.4 (2)	C23—C28—H28	120.00
C21—C23—C24	122.5 (3)	C27—C28—H28	120.00
C21—C23—C28	119.5 (3)	C26—C29—H29A	109.00
C24—C23—C28	118.0 (3)	C26—C29—H29B	109.00
C23—C24—C25	120.9 (3)	C26—C29—H29C	109.00
C24—C25—C26	121.8 (3)	H29A—C29—H29B	109.00
C25—C26—C27	117.4 (4)	H29A—C29—H29C	109.00
C25—C26—C29	121.4 (4)	H29B—C29—H29C	110.00
C12—O11—C10—C6	179.6 (3)	C1—C6—C10—O11	147.6 (3)
C12—O11—C10—C14	−0.8 (3)	C1—C6—C10—C14	−31.9 (5)
C10—O11—C12—C13	0.2 (3)	C5—C6—C10—O11	−32.0 (4)
C10—O11—C12—C15	−176.0 (3)	C5—C6—C10—C14	148.5 (4)
O8—N7—C5—C4	129.4 (3)	O11—C10—C14—C13	1.0 (4)
O8—N7—C5—C6	−47.1 (4)	C6—C10—C14—C13	−179.5 (3)

O9—N7—C5—C4	−48.9 (5)	O11—C12—C13—C14	0.4 (4)
O9—N7—C5—C6	134.6 (4)	C15—C12—C13—C14	175.6 (3)
C15—N16—N20—C21	0.7 (4)	O11—C12—C15—N16	−67.3 (3)
C17—N16—N20—C21	−169.8 (3)	O11—C12—C15—C22	48.1 (4)
N20—N16—C15—C12	121.0 (3)	C13—C12—C15—N16	117.7 (4)
N20—N16—C15—C22	−1.7 (3)	C13—C12—C15—C22	−126.9 (4)
C17—N16—C15—C12	−68.8 (4)	C12—C13—C14—C10	−0.8 (4)
C17—N16—C15—C22	168.5 (3)	N16—C15—C22—C21	1.9 (3)
N20—N16—C17—O19	176.2 (3)	C12—C15—C22—C21	−120.3 (3)
N20—N16—C17—C18	−4.7 (5)	N20—C21—C22—C15	−1.8 (4)
C15—N16—C17—O19	6.8 (5)	C23—C21—C22—C15	178.7 (3)
C15—N16—C17—C18	−174.0 (3)	N20—C21—C23—C24	1.1 (5)
N16—N20—C21—C22	0.8 (4)	N20—C21—C23—C28	−179.9 (3)
N16—N20—C21—C23	−179.7 (3)	C22—C21—C23—C24	−179.4 (3)
C6—C1—C2—C3	0.4 (6)	C22—C21—C23—C28	−0.4 (5)
C2—C1—C6—C5	−0.3 (5)	C21—C23—C24—C25	179.0 (3)
C2—C1—C6—C10	−180.0 (3)	C28—C23—C24—C25	−0.1 (5)
C1—C2—C3—C4	−0.1 (6)	C21—C23—C28—C27	−178.5 (3)
C2—C3—C4—C5	−0.3 (6)	C24—C23—C28—C27	0.6 (5)
C3—C4—C5—N7	−176.0 (3)	C23—C24—C25—C26	−0.8 (6)
C3—C4—C5—C6	0.4 (5)	C24—C25—C26—C27	1.1 (6)
N7—C5—C6—C1	176.1 (3)	C24—C25—C26—C29	−178.6 (4)
N7—C5—C6—C10	−4.2 (4)	C25—C26—C27—C28	−0.5 (6)
C4—C5—C6—C1	−0.1 (4)	C29—C26—C27—C28	179.1 (4)
C4—C5—C6—C10	179.6 (3)	C26—C27—C28—C23	−0.3 (6)

Hydrogen-bond geometry (Å, °)

Cg4 is the centroid of the C23—C28 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C14—H14···O19 ⁱ	0.93	2.56	3.462 (4)	162
C18—H18C···Cg4 ⁱⁱ	0.96	2.69	3.595 (4)	158

Symmetry codes: (i) $-x, -y, -z+2$; (ii) $-x, -y, -z+1$.